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Crystal-field effect on magnetic ordering temperature of collinear antiferromagnet

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The correlated effective field approach, proposed by Lines, for computing the magnetic ordering temperature of a ferromagnet with single-ion anisotropy, is generalized for the case of a collinear uniaxial antiferromagnet. The dependence of the Néel temperature T_N on the DS_z^2-type crystal field anisotropy parameter D is obtained numerically for lattices of cubic and tetragonal symmetry. For the latter case the influence of lowering the interaction dimensionality on T_N is presented for the spin quantum numbers $S = 1$ and $7/2$.

1. Introduction

The influence of a crystal electric field on the phase transition temperature of Heisenberg magnets is an important problem for many magnetic materials, especially when the thermal energy, exchange interaction and crystal-field splitting energies are of the same order of magnitude. Among others (see, for example, refs. [1,2]), the correlated effective field (CEF) theory by Lines [3,4] has the advantage that with modest computational efforts the magnetic transition temperature T_c can be obtained numerically for a complete range of crystal-field anisotropy to Heisenberg nearest-neighbor exchange ratio $-\infty < D/J < \infty$, thus including easy-axis and easy-plane types of ordering, and for the arbitrary physically relevant spin value $1 \le S \le 7/2$. The deviation of CEF results for T_c from the best known ones obtained by high-temperature-series expansions and a self-consistent Green's function approach does not exceed 12% for spin value $S = 1$ and has a tendency to decrease with increasing S value (see the discussion in ref. [4] and references therein). But as was pointed out by Lines [4], his equations (2.2) and (2.10) for the computation of the magnetic transition temperature T_c are applicable only for the ferromagnetic type of ordering, because one arrives at a negative value of T_c when simple reversing the sign of the exchange J in them.

In this paper we generalize the CEF theory for a two-sublattice collinear uniaxial antiferromagnet and compute the Néel antiferromagnetic temperature of a magnet with a DS_z^2-type crystal-field anisotropy as a function of D/J for the set of spin values from 1 to 7/2.

2. CEF theory for a two-sublattice antiferromagnet

Consider a two-sublattice collinear antiferromagnet with Hamiltonian to be assumed in the form

$$\mathscr{H} = \sum_i \mathscr{H}_i^{CF} + \mathscr{H}_{ex}, \qquad (1)$$

where $\mathscr{H}_i^{CF}$ characterizes the single-ion crystal-field anisotropy. The eigenvalues and eigenfunctions are assumed to be known. We choose the

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